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On the numerical study of deep conducting lamellar diffraction gratings

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Abstract. A root-finding algorithm for the solution of the eigenvalue equation linked with the theoretical study of lossy lamellar gratings is outlined. The computation time seems to be shorter than required when using a method proposed by Botten *et al.* (1981). The agreement is found to be excellent.

The study of deep lamellar gratings invariably involves the numerical determination of the roots of a transcendental equation [1]. In this paper such a determination is carried out, using a method completely different from the one proposed by Botten *et al.* [2].

The notation (figure 1) is slightly different from that used in [2]; it is the same as used in [1] except that the refractive index of medium 2 is here denoted by ν instead of ν_2. The problem is to find the values of ρ† for which

$$f(\rho,\nu,\theta)=\cos(\alpha_0 d)-\cos(\beta c)\cos(\gamma e)+\frac{1}{2}\left(q\frac{\beta}{\gamma}+\frac{1}{q}\frac{\gamma}{\beta}\right)\sin(\beta c)\sin(\gamma e)=0, \tag{1}$$

where

$$k_0=\omega(\varepsilon_0\mu_0)^{1/2},\quad \alpha_0=k_0\nu_1\sin\theta, \tag{2}$$

$$\beta=(k_0^2\nu_1^2-\rho)^{1/2},\quad \gamma=(k_0^2\nu^2-\rho)^{1/2}, \tag{3}$$

$$q=\begin{cases}1 & \text{for P polarization,}\\ \nu^2/\nu_1^2 & \text{for S polarization.}\end{cases} \tag{4}$$

Since ν, ρ, β and γ as considered here are complex numbers, so the square-root expressions must be precisely defined: $z=Z^{1/2}$ is taken to mean that $z^2=Z$ and $\operatorname{Re} z+\operatorname{Im} z\geqslant 0$ so that, if Z is real, either $Z^{1/2}$ or $Z^{1/2}/i$ is real and positive.

Whereas the method used in [2] (which relies on the theory of analytic functions) is, to a certain extent, general, our treatment is more specific. It is necessary that, for a particular combination of the parameters ν and θ, an efficient method is available for finding the roots of equation (1); the combination turns out to be $\theta=0$ and ν real (a lossless dielectric grating illuminated in normal incidence), as shown in [1] and briefly explained below.

† Botten *et al.* [2] approached the problem by seeking to evaluate β, as defined here by equation (3).

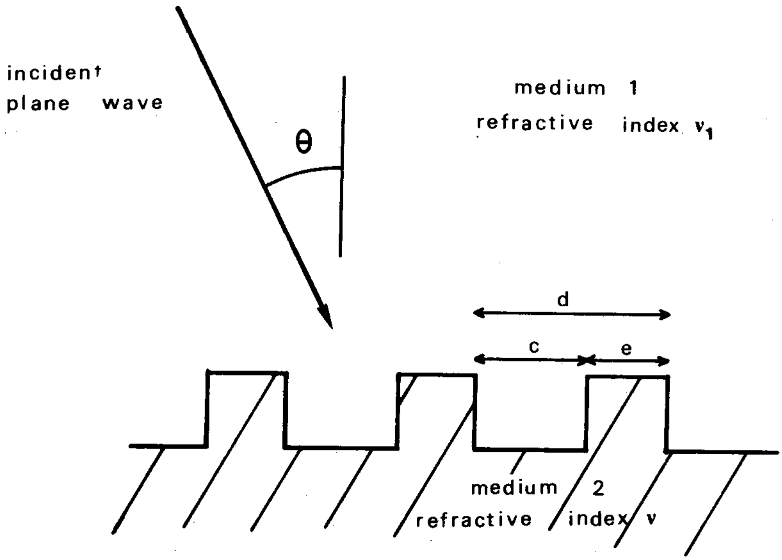

Figure 1. A lamellar grating illuminated by a plane wave.

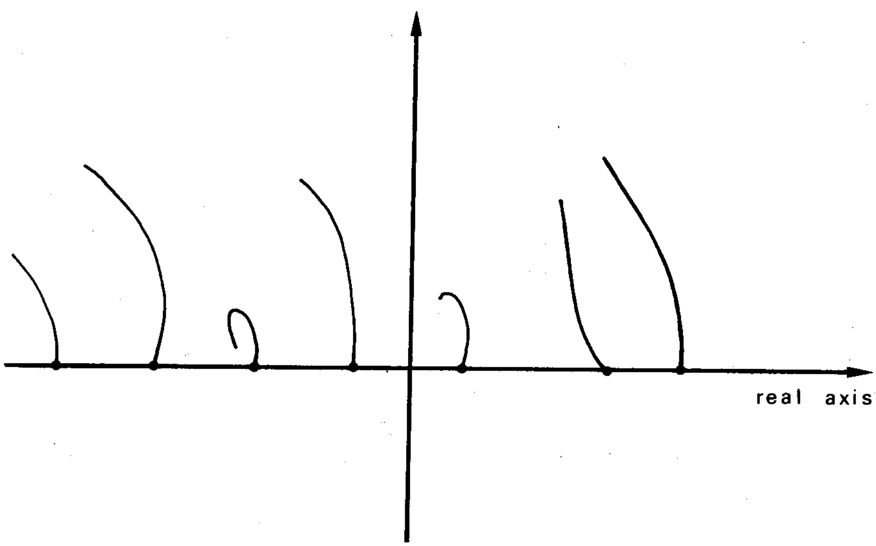

Figure 2. Schematic representation of the roots' trajectories in the complex plane. The points on the real axis are the roots $\rho_n(0)$, the eigenvalues of $\mathscr{L}$ *for* $\nu=\nu_0$ and $\theta=0$. When t varies, these roots move in the complex plane. A curve is the trajectory corresponding to a fixed n.

It must be kept in mind that the roots we are looking for are the eigenvalues of a certain operator ($\mathscr{L}$ in [1]). When ν is a real number ν_0, $\mathscr{L}$ is a self-adjoint operator and consequently its eigenvalues are real. They are located on the real axis of the ρ complex plane (figure 2), and it is easy to compute a number (say N) of them, especially if the grating is illuminated in normal incidence. Indeed, the function $f(\rho, \nu_0, 0)$ is then [1] the product of two functions $f_e(\rho, \nu_0)$ and $f_o(\rho, \nu_0)$†, both having

† The roots of f_e and f_o are associated with, respectively, even and odd eigenfunctions of $\mathscr{L}$.

'separable roots'. This means that we are able to divide the real axis into intervals, each containing one and only one root. For the purposes of numerical calculation this is, of course, ideal.

Unfortunately, if ν is complex $\mathscr{L}$ is not a self-adjoint operator and its eigenvalues can be complex, which makes them much more difficult to determine. Let us introduce two monotonic functions $\phi(t)$ and $\psi(t)$ of a parameter t varying on $(0, 1)$, and defined such that

$$\phi(0)=\nu_0 \text{ (real)}, \quad \phi(1)=\nu \text{ (complex)},$$
$$\psi(0)=0, \qquad \psi(1)=\theta.$$

When we substitute ν and θ for $\phi(t)$ and $\psi(t)$, respectively, in $f(\rho, \nu, \theta)$, we define a function $F(\rho, t)$ of two independent variables:

$$f(\rho, \phi(t), \psi(t))=F(\rho, t). \tag{5}$$

For each value of t, let us consider N roots $\rho_n(t)$ of the equation $F(\rho, t)=0$. We assume that $\rho_n(t)$ are continuous and differentiable functions (figure 2). Then, for fixed n, use of the differential equation

$$\frac{d\rho_n}{dt}=G(\rho_n, t), \tag{6}$$

with

$$G(\rho, t)=-\frac{\partial F}{\partial t}\bigg/\frac{\partial F}{\partial \rho} \tag{7}$$

(see the Appendix) enables $\rho_n(1)$ to be determined from a knowledge of $\rho_n(0)$. Taking into account the fact that $G(\rho_n, t)$ is complicated, equation (6) has to be integrated numerically using a computer. We used the classical fourth-order Runge–Kutta method but, *a priori*, any standard algorithm can be used. Owing to the inevitable errors associated with any numerical process, we obtain only estimates $\tilde{\rho}_n(1)$. If necessary, better accuracy can be achieved by using any of the classical methods for the numerical solution of equations. The method used here is an adaptation to the complex domain of the method of 'false position'. The iteration is initiated by taking $\tilde{\rho}_n(1)$ and $\tilde{\rho}_n(1-h)$ as approximate values of $\rho_n(1)$ (h standing for the integration spacing).

In order to compare the two methods we have carried out computations using the parameters from the third test proposed by Botten *et al.*[3]:

$$d=1{\cdot}0, \quad c=0{\cdot}4, \quad e=0{\cdot}6, \quad \lambda=0{\cdot}55, \quad \nu_1=1{\cdot}0, \quad \nu=0{\cdot}756+i2{\cdot}462, \quad \theta=5°,$$

for P polarization. Excellent agreement is obtained, the results being all the same to nine significant figures. The computing time for this example was about 3 s on an IBM 3081-D computer, whereas Botten *et al.* report a time of 30 s on a CDC Cyber 170/730. Consequently we are now employing the method described in this paper in our own studies of lossy lamellar gratings. As an illustration, figure 3 shows the eigenvalue trajectories for an example more academic than practical. It is interesting to observe what happens to the 'pairs of roots' when, for a fixed incidence $\theta=0$, the imaginary part of the refractive index increases linearly from 0 to 4. The least that can be said is that the behaviour is not simple!

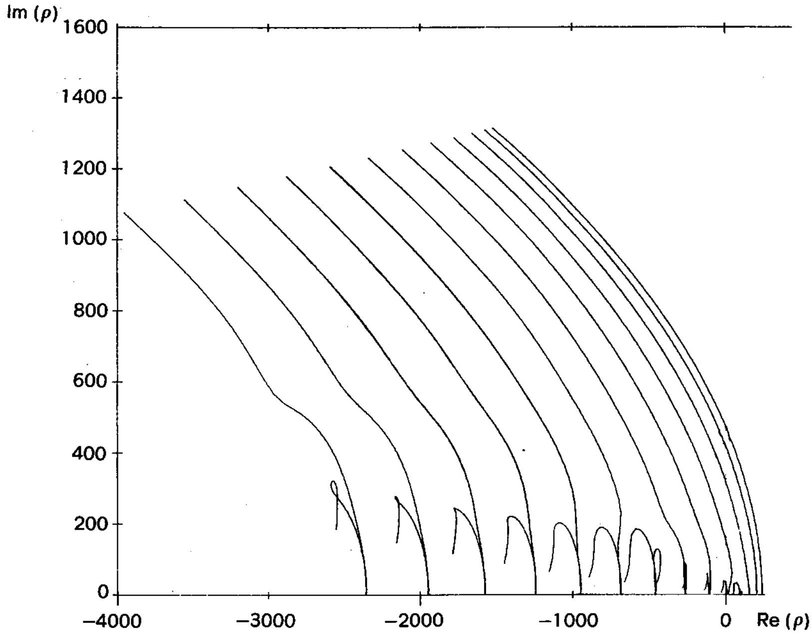

Figure 3. The trajectories of 25 eigenvalues $\rho_n(t)$ for normal incidence (the trajectories of the other eigenvalues all start from smaller real values) for the parameters $d=1{\cdot}5$, $e=c=0{\cdot}75$, $\lambda=0{\cdot}6$, $\theta=0$, $v_1=1{\cdot}0$, $v_0=1{\cdot}5$, $v=1{\cdot}5+i4$ and P polarization. A few trajectories that stay very close to the real axis are not shown clearly.

In conclusion, as part of continuing theoretical studies of deep lossy lamellar gratings, we have tried in this short paper to present a numerical algorithm for the solution of the eigenvalue equation. The numerical experiments reported demonstrate that the method is successful in determining the roots of the transcendental equation, being in excellent agreement with the earlier method of Botten *et al.* [2] but requiring apparently a significantly shorter computation time. The results of this work thus represent an advance in the use of the practically important eigenvalue method [4, 5], a method which allows one to deal with lamellar gratings for which the ratio of the groove depth to the period is of the order of several hundreds [4–6].

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Appendix

The expression $G(\rho, t)$ when ϕ and ψ are linear functions of t

Combining equations (1) and (5) gives

$$f(\rho, \phi(t), \psi(t)) = \cos(k_0 d v_1 \sin\psi(t)) - \cos(\beta c)\cos(\gamma e) + \frac{1}{2}\left(q\frac{\beta}{\gamma} + \frac{1}{q}\frac{\gamma}{\beta}\right)\sin(\beta c)\sin(\gamma e) = 0.$$

Using the relations $\phi(t) = v_0 + (v - v_0)t$ and $\psi(t) = \theta t$, and setting

$$q = \frac{\phi(t)^2}{v_1^2}, \quad \beta = (k_0^2 v_1^2 - \rho)^{1/2}, \quad \gamma = (k_0^2 \phi^2(t) - \rho)^{1/2},$$

we obtain

$$G(\rho, t) = -\frac{\dfrac{\partial F}{\partial t}}{\dfrac{\partial F}{\partial \rho}} = -\frac{\dfrac{\partial f}{\partial \psi}\dfrac{d\psi}{dt} + \dfrac{\partial f}{\partial \gamma}\dfrac{\partial \gamma}{\partial t} + \dfrac{\partial f}{\partial \phi}\dfrac{d\phi}{dt}}{\dfrac{\partial f}{\partial \beta}\dfrac{\partial \beta}{\partial \rho} + \dfrac{\partial f}{\partial \gamma}\dfrac{\partial \gamma}{\partial \rho}},$$

where

$$\frac{\partial f}{\partial \psi} = -k_0 v_1 d \sin(k_0 d v_1 \sin \psi(t)) \cos \psi(t),$$

$$\frac{d\psi}{dt} = \theta,$$

$$\frac{\partial f}{\partial \gamma} = e \cos(\beta c) \sin(\gamma e) + \frac{1}{2}\left(-\frac{q\beta}{\gamma^2} + \frac{1}{q\beta}\right) \sin(\beta c) \sin(\gamma e) + \frac{e}{2}\left(\frac{q\beta}{\gamma} + \frac{\gamma}{q\beta}\right) \sin(\beta c) \cos(\gamma e),$$

$$\frac{\partial f}{\partial \beta} = c \sin(\beta c) \cos(\gamma e) + \frac{1}{2}\left(\frac{q}{\gamma} - \frac{\gamma}{q\beta^2}\right) \sin(\beta c) \sin(\gamma e) + \frac{c}{2}\left(\frac{q\beta}{\gamma} + \frac{\gamma}{q\beta}\right) \cos(\beta c) \sin(\gamma e),$$

$$\frac{\partial \gamma}{\partial t} = \frac{1}{2\gamma}\frac{\partial}{\partial t}(k_0^2 \phi^2(t) - \rho) = \frac{k_0^2}{\gamma}(v - v_0)\phi(t),$$

$$\frac{\partial f}{\partial \phi} = \left(\frac{\beta}{\gamma}\frac{\phi(t)}{v_1^2} - \frac{\gamma}{\beta}\frac{v_1^2}{\phi^3(t)}\right) \sin(\beta c) \sin(\gamma e),$$

$$\frac{d\phi}{dt} = v - v_0,$$

$$\frac{\partial \beta}{\partial \rho} = -\frac{1}{2\beta},$$

$$\frac{\partial \gamma}{\partial \rho} = -\frac{1}{2\gamma}.$$

References

[1] SURATTEAU, J. Y., CADILHAC, M., and PETIT, R., 1983, *J. Optics, Paris*, **14,** 273–288.

[2] BOTTEN, L. C., CRAIG, M. S., and MCPHEDRAN, R. C., 1981, *Optica Acta*, **28,** 1103–1106.

[3] BOTTEN, L. C., CRAIG, M. S., and MCPHEDRAN, R. C., 1983, *Comput. Phys. Commun.*, **29,** 245–259.

[4] BOTTEN, L. C., CRAIG, M. S., MCPHEDRAN, R. C., ADAMS, J. L., and ANDREWARTHA, J. R., 1981, *Optica Acta*, **28,** 413–428.

[5] BOTTEN, L. C., CRAIG, M. S., MCPHEDRAN, R. C., ADAMS, J. L., and ANDREWARTHA, J. R., 1981, *Optica Acta*, **28,** 1087–1102.

[6] PETIT, R., SURATTEAU, J. Y., CADILHAC, M., 1984, *Application, Theory and Fabrication of Periodic Structures, Diffraction Gratings and Moiré Phenomena II*, SPIE Proc. VA. 503 (Bellingham: SPIE), Chap. 5.